Conservation of the spectral moments
in the n-pole approximation

F. Mancini[*]

Dipartimento di Scienze Fisiche "E.R. Caianiello" e Unità I.N.F.M. di Salerno

Università di Salerno, 84081 Baronissi (SA), Italy

Abstract

A formulation of the Green's function method is presented in the n-pole approximation. Without referring to a specific model we give a general scheme of calculations that easily permits the computation of the "single-particle" Green's function in terms of the energy matrix. A theorem is proved which states that the moments of the spectral density function are conserved up to the order $2(n-l+1)$, where l is the order of the composite field. A comparison with the spectral density approach is also discussed.

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[*]Corresponding author. E-mail address: mancini@vaxsa.csied.unisa.it

The theoretical analysis of highly correlated electron systems contains many unsolved problems and a complete and systematic formulation is still lacking. Many analytical methods have been developed. Among many we recall the slave boson method [1], the non-crossing approximation [2], the d_∞ method [3], the projection operator method [4], the method of equation of motion [5], the spectral density approach [6], the coherent potential approximation [7], the composite operator method [8]. It is not easy to judge the reliability of the various approximations. Certainly, one important aspect is the capability to conserve the symmetries inherent to the model and some relations, which can be derived on general basis.

A scheme of approximation, common to various methods [4-6, 8], is the so called n-pole approximation, based on a linearization of the equations of motion. In this article we show that in this scheme the exact relation between the spectral moments and the spectral density is conserved: *(i)* at any order when the moments are calculated with respect to the linearized equations: *(ii)* up to the order $2(n-l+1)$, where l is the order of the composite field, when calculated with respect to the full equations of motion. This aspect is attractive and shows that the approximation can reproduce some essential features of the single-particle function.

Let us consider a certain Hamiltonian

$$H = H(\phi_1, \ldots, \phi_p) \tag{1}$$

the set $\{\phi_i\}$ denotes field operators. In order to close the infinite hierarchy of equations of motion some truncation is necessary. One procedure is to choose a basis of operators $\{\psi_1, \ldots, \psi_n\}$ and linearize the equations of motion as

$$i\frac{\partial}{\partial t}\psi(x) = [\psi(x), H] = \epsilon(-i\vec{\nabla})\psi(x) + \delta j(x) \approx \epsilon(-i\vec{\nabla})\psi(x) \tag{2}$$

where the eigenvalue or energy matrix ϵ [9] is self-consistently calculated by means of the equation

$$\epsilon(-i\nabla_x)\langle\left[\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{y}, t)\right]_\pm\rangle = \langle\left[[\psi(\mathbf{x}, t), H]\,\psi^\dagger(\mathbf{y}, t)\right]_\pm\rangle \tag{3}$$

The symbol $[\ldots]_\pm$ denotes equal-time anticommutator or commutator, in dependence of the statistics of the set $\{\psi_i\}$. The rank of the energy matrix is equal to n, the number of

components of the vector $\psi(x)$. When the basis $\{\psi_i\}$ coincides with the original set $\{\phi_i\}$, the linearization procedure given in Eq. (2) corresponds to the Hartree-Fock approximation. The fields ψ_i may be called composite fields [8], since they are generally constructed as a combination of the original fields ϕ_i.

Let us consider the thermal retarded Green's function [10]

$$S(x,y) = \langle R\left[\psi(x)\psi^\dagger(y)\right]\rangle = \frac{i}{(2\pi)^{d+1}} \int d^d k d\omega e^{i\mathbf{k}\cdot(\mathbf{x}\cdot\mathbf{y})-i\omega(t_x-t_y)} S(\mathbf{k},\omega) \tag{4}$$

where R is the usual retarded operator and the symbol $\langle \ldots \rangle$ denotes the thermal average. d is the dimensionality of the system. By means of the Heisenberg equation (2), in the linearized form, the Fourier transform $S(\mathbf{k},\omega)$ is given by

$$S(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon(\mathbf{k})} I(\mathbf{k}) = \frac{1}{D(\mathbf{k},\omega)} \sum_{i=0}^{n-1} \omega^i \lambda^{(i)}(\mathbf{k}) \tag{5}$$

where

$$I(\mathbf{k}) = F.T.\langle\left[\psi(\mathbf{x},t),\psi^\dagger(\mathbf{y},t)\right]_\pm\rangle \tag{6}$$

the symbol $F.T.$ denoting the Fourier transform, and

$$D(\mathbf{k},\omega) = \sum_{i=0}^{n} \omega^i a_i(\mathbf{k}) \tag{7}$$

is the characteristic polynomial of the matrix $\epsilon(\mathbf{k})$. The characteristic coefficients $a_i(\mathbf{k})$ are defined by the following relation

$$a_{n-k}(\mathbf{k}) = (-1)^k Tr_k[\epsilon(\mathbf{k})] \qquad \text{for} \quad 0 \leq k \leq n \tag{8}$$

Where $Tr_k[\epsilon]$ is the trace of the k'th order, defined as the sum of the determinants of all $\binom{n}{k}$ matrices of order $(k \times k)$ that can be formed by intersecting any k rows of ϵ with the same k columns. We note that $Tr_n[\epsilon] = Det[\epsilon]$ and the convention $Tr_0[\epsilon] = 1$ is used. The $\lambda^{(i)}(\mathbf{k})$ are the $n \times n$ matrices, determined by the equation

$$\sum_{i=0}^{n-1} \omega^i \lambda^{(i)}(\mathbf{k}) = D(\mathbf{k},\omega)\left[\omega - \epsilon(\mathbf{k})\right]^{-1} I(\mathbf{k}) \tag{9}$$

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The solution of this equation gives:

$$\lambda^{(m)}(\mathbf{k}) = \sum_{s=m+1}^{n} a_s(\mathbf{k})\epsilon^{s-m-1}(\mathbf{k})I(\mathbf{k}) \qquad \text{for} \quad 0 \le m \le n-1 \tag{10}$$

The Green's function (5) has a n-pole structure

$$S(\mathbf{k},\omega) = \sum_{i=1}^{n} \frac{\sigma^{(i)}(\mathbf{k})}{\omega - E_i(\mathbf{k}+i\eta)} \tag{11}$$

The energy spectra $E_i(\mathbf{k})$ are the characteristic values of the matrix $\epsilon(\mathbf{k})$ and correspond to the zeros of the characteristic polynomial

$$\sum_{m=0}^{n} a_m(\mathbf{k})E_i^m(\mathbf{k}) = 0 \tag{12}$$

The spectral functions are given by

$$\sigma^{(i)}(\mathbf{k}) = \frac{1}{b_i(\mathbf{k})} \sum_{m=0}^{n-1} E_i^m(\mathbf{k})\lambda^{(m)}(\mathbf{k}) \tag{13}$$

where we put

$$b_i(\mathbf{k}) = \prod_{j=1,j\neq i}^{n} [E_i(\mathbf{k}) - E_j(\mathbf{k})] \tag{14}$$

We also note that in the n-pole expansion, the Green's function can be expressed as

$$S_{\alpha\beta}(\mathbf{k},\omega) = \frac{I_{\alpha\beta}(\mathbf{k})}{\omega - \Sigma_{\alpha\beta}(\mathbf{k},\omega)} \tag{15}$$

where the self energy $\Sigma_{\alpha\beta}(\mathbf{k},\omega)$ is given by

$$\Sigma_{\alpha\beta}(\mathbf{k},\omega) = \frac{1}{\sum_{i=0}^{n-1}\omega^i\lambda_{\alpha\beta}^{(i)}(\mathbf{k})} \sum_{i=0}^{n-1} \omega^i[\epsilon(\mathbf{k})\lambda^{(i)}(\mathbf{k})]_{\alpha\beta} \tag{16}$$

Summarizing, in this scheme of approximation the calculation of the Green's function requires the following steps:

(i) Given a certain Hamiltonian, a basic set $\{\psi_i\}$ of field operators is chosen;

(ii) the energy matrix $\epsilon(\mathbf{k})$ is calculated by means of Eq. (3);

(iii) the energy spectra $E_i(\mathbf{k})$ are calculated as the roots of the characteristic polynomial of $\epsilon(\mathbf{k})$;

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(iv) the $\lambda^{(i)}(\mathbf{k})$ matrices are calculated in terms of the energy matrix $\epsilon(\mathbf{k})$ by means of Eq. (10).

We want now to study if the n-pole approximation conserves the exact relation between the spectral moments and the spectral density, that can be derived on general basis. We start by the following definition for the spectral moments

$$M^{(k)}(\mathbf{k}) = F.T. \left[\left(\frac{i\partial}{\partial t_x} \right)^{k-p} \left(-\frac{i\partial}{\partial t_y} \right)^{p} \langle \left[\psi(x), \psi^{\dagger}(y) \right]_{\pm} \rangle \right]_{t_x=t_y} \qquad \text{[for } 0 \le p \le k] \qquad (17)$$

We note that $M^{(k)}(\mathbf{k})$ is a $n \times n$ matrix and is a generalization of the quantity usually introduced in the literature, where the spectral moments are referred to the one-particle propagator. Let us introduce the spectral density function $A(\mathbf{k}, \omega)$

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} Im S(\mathbf{k}, \omega + i\eta) \qquad (18)$$

and consider the quantity

$$B^{(k)}(\mathbf{k}) = \int_{-\infty}^{+\infty} d\omega \omega^k A(\mathbf{k}, \omega) \qquad (19)$$

By taking time derivatives of Eq. (4) we find the following relation between the spectral moments and the spectral density

$$M^{(k)}(\mathbf{k}) = B^{(k)}(\mathbf{k}) \qquad (20)$$

This relation is an exact one and must hold for any integer non negative value of k. By means of the field equation Eq. (2) the spectral moments can be written as

$$M^{(k)}(\mathbf{k}) = \tilde{M}^{(k)}(\mathbf{k}) + \delta M^{(k)}(\mathbf{k}) \qquad (21)$$

where

$$\tilde{M}^{(k)}(\mathbf{k}) = \epsilon^k(\mathbf{k}) I(\mathbf{k}) \qquad (22)$$

$$\delta M^{(0)}(\mathbf{k}) = \delta M^{(1)}(\mathbf{k}) = 0 \qquad (23)$$

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$$\delta M^{(k)}(\mathbf{k}) = \sum_{m=1}^{k-1} F.T. \left[\epsilon^{k-m-1}(i\partial/\partial t_x)^m \langle [\delta j(x), \psi^\dagger(y)]_\pm \rangle \right]_{t_x=t_y} \qquad [\text{for} \quad k \geq 2] \qquad (24)$$

What see that the $\tilde{M}^{(k)}(\mathbf{k})$ correspond to the spectral moments calculated in the n-pole approximation, where the higher order field $\delta j(x)$ in the Heisenberg equation (2) is neglected. We will now prove that the spectral moments $\tilde{M}^{(k)}(\mathbf{k})$ satisfy the relation

$$\tilde{M}^{(k)}(\mathbf{k}) = \int_{-\infty}^{+\infty} d\omega \omega^k A(\mathbf{k}, \omega) \qquad \text{for any} \quad k \qquad (25)$$

The proof is divided in two steps: (i) $\tilde{M}^{(k)}(\mathbf{k})$ and $B^{(k)}(\mathbf{k})$ satisfy for $k \geq n$ the same recurrence relation; (ii) the equality $\tilde{M}^{(k)}(\mathbf{k}) = B^{(k)}(\mathbf{k})$ is satisfied for $k \leq n$.

By recalling that $a_s(\mathbf{k})$ are the coefficients of the characteristic polynomial of the matrix $\epsilon(\mathbf{k})$, the Hamilton-Cayley theorem says

$$\sum_{s=0}^{n} a_s(\mathbf{k}) \epsilon^s(\mathbf{k}) = 0 \qquad (26)$$

Then, the moments $\tilde{M}^{(k)}(\mathbf{k})$ satisfy the recurrence relation

$$\tilde{M}^{n+k}(\mathbf{k}) = -\sum_{s=0}^{n-1} a_s(\mathbf{k}) \tilde{M}^{s+k}(\mathbf{k}) \qquad \text{for} \quad k \geq 0 \qquad (27)$$

On the other hand, by noting that from Eq. (11) the spectral density is given by $A(\mathbf{k}, \omega) = \sum_{i=1}^{n} \sigma^{(i)}(\mathbf{k}) \delta [\omega - E_i(\mathbf{k})]$, we have

$$B^{(k)}(\mathbf{k}) = \sum_{i=1}^{n} E_i^k(\mathbf{k}) \sigma^{(i)}(\mathbf{k}) \qquad (28)$$

Since the $E_i(\mathbf{k})$ satisfy the relation

$$E_i^{n+k}(\mathbf{k}) = -\sum_{m=0}^{n-1} a_m(\mathbf{k}) E_i^{m+k}(\mathbf{k}) \qquad \text{for} \quad k \geq 0 \qquad (29)$$

the quantities $B^{(k)}(\mathbf{k})$ satisfy the recurrence relation

$$B^{(n+k)}(\mathbf{k}) = -\sum_{m=0}^{n-1} a_m(\mathbf{k}) B^{(m+k)}(\mathbf{k}) \qquad \text{for} \quad k \geq 0 \qquad (30)$$

We see that the spectral moments $\tilde{M}^{(k)}(\mathbf{k})$ and the quantities $B^{(k)}(\mathbf{k})$ satisfy the same recurrence relation for $k \geq n$. To show that they coincide, it is enough to consider the case $0 \leq k \leq n$.

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Let us take $1 \le k \le n-1$. By means of the expression (13) for the spectral functions we can write

$$B^{(k)}(\mathbf{k}) = \sum_{m=0}^{n-1} \lambda^{(m)}(\mathbf{k}) P^{(k+m)}(\mathbf{k}) \tag{31}$$

where we have defined

$$P^{(k)}(\mathbf{k}) \equiv \sum_{i=1}^{n} \frac{E_i^k(\mathbf{k})}{b_i(\mathbf{k})} \tag{32}$$

By means of the relation (29) the quantities $P^{(k)}(\mathbf{k})$ satisfy the recurrence relation

$$\sum_{m=0}^{n} a_m(\mathbf{k}) P^{m+k}(\mathbf{k}) = 0 \qquad \text{for} \quad k \ge 0 \tag{33}$$

By simple algebraic relations it is easy to show that

$$P^{(k)}(\mathbf{k}) = \begin{cases} 0 & \text{for} \quad 0 \le k \le n-2 \\ 1 & \text{for} \quad k = n-1 \end{cases} \tag{34}$$

By recalling that from Eq. (10) $\lambda^{(m)} = \epsilon \lambda^{(m+1)} + a_{m+1} I$ we can then write

$$B^{(k)}(\mathbf{k}) = \lambda^{(n-1)}(\mathbf{k}) P^{(k+n-1)}(\mathbf{k}) + \epsilon(\mathbf{k}) \sum_{m=n-1-k}^{n-2} \lambda^{(m+1)}(\mathbf{k}) P^{(k+m)}(\mathbf{k}) \tag{35}$$

$$+ I(\mathbf{k}) \sum_{m=n-1-k}^{n-2} a_{m+1}(\mathbf{k}) P^{(k+m)}(\mathbf{k}) \tag{36}$$

On the other hand $\lambda^{(n-1)}(\mathbf{k}) = a_n I(\mathbf{k})$, therefore the previous expression takes the form

$$B^{(k)}(\mathbf{k}) = \epsilon(\mathbf{k}) B^{(k-1)}(\mathbf{k}) + I(\mathbf{k}) \sum_{m=n-1-k}^{n-1} a_{m+1}(\mathbf{k}) P^{(k+m)}(\mathbf{k}) = \epsilon(\mathbf{k}) B^{(k-1)}(\mathbf{k}) \tag{37}$$

where the relation (33) for $k \ge 1$ has been used. But for $k = 0$ it is easy to see that $B^{(0)}(\mathbf{k}) = I(\mathbf{k})$, therefore

$$B^{(k)}(\mathbf{k}) = \epsilon^k(\mathbf{k}) I(\mathbf{k}) = \tilde{M}^{(k)}(\mathbf{k}) \qquad \text{for} \quad 0 \le k \le n-1 \tag{38}$$

Because of the recurrence relations (27) and (30), the equality (38) holds also for $k = n$ and the step (ii) is thus proved. Then, the equality $\tilde{M}^{(k)}(\mathbf{k}) = B^{(k)}(\mathbf{k})$ is true for any k and the relation (25) is demonstrated.

We now turn to the more general question if the n-pole approximation conserves the full spectral moments $M^{(k)}(\mathbf{k})$, calculated by the exact Heisenberg equations. In the context of the Hubbard model it is known that in the 2-pole approximation the first 4 spectral moments relative to the electronic field are conserved [6,11]. For higher order moments the situation is not known.

It is always possible to choose the basic set as

$$i\frac{\partial}{\partial t}\psi_l(x) = [\psi_l(x), H] = \sum_{p=1}^{l+1}\gamma_{lp}(-i\nabla)\psi_p(x) \qquad [\text{for } 1 \leq l \leq n-1] \qquad (39)$$

For this choice we have that

$$\begin{aligned} \epsilon_{lp} &= \gamma_l p \\ \delta j_l &= 0 \end{aligned} \qquad \text{for } 1 \leq l, p \leq n-1 \qquad (40)$$

and the matrix ϵ has the following structure

$$\epsilon_{lp} = 0 \quad \text{for} \begin{cases} l \leq n-2 \\ p \geq l+2 \end{cases} \qquad (41)$$

From the definition (24) and by use of the exact Heisenberg equation (38) we can derive the following recurrence relation

$$\delta M_{lp}^{(k)}(\mathbf{k}) = \epsilon_{lr}(\mathbf{k})\delta M_{rs}^{(k-2)}(\mathbf{k})\epsilon_{sp}^{\dagger}(\mathbf{k}) \qquad \text{for } 1 \leq l, p \leq n-1 \qquad (42)$$

Then, by means of Eqs. (24) and (40) we find that the matrix $\delta M^{(k)}(\mathbf{k})$ has the following property

$$\delta M_{lp}^{(2k)}(\mathbf{k}) = \delta M_{lp}^{(2k+1)}(\mathbf{k}) = 0 \qquad \text{for } 1 \leq l, p \leq n-k \qquad (43)$$

By recalling Eq. (25) we can then enunciate the following theorem.

Given a set of fields $\{\psi_l, l = 1, \ldots, n\}$, if the subset $\{\psi_l, l = 1, \ldots, n-1\}$ satisfies linear Heisenberg equations $i\,(\partial/\partial t)\,\psi_l(x) = \sum_{p=1}^{l+1}\gamma_{lp}(-i\nabla)\psi_p(x)$, then the first $2(n-l+1)$ spectral moments for the fields ψ_l $[1 \leq l \leq n-1]$ are conserved [12].

The theorem proved in this article shows that the n-pole approximation is equivalent to the SDA [6], when the polar ansatz is considered. The following remark is worth to be

mentioned. In the SDA the unknown quantities, the energy spectra $E_i(\mathbf{k})$ and the spectral functions $\sigma^{(i)}(\mathbf{k})$, are evaluated in terms of the spectral moments through the equation

$$M^{(k)}(\mathbf{k}) = \sum_{i=1}^{n} E_i^k(\mathbf{k}) \sigma^{(i)}(\mathbf{k}) \tag{44}$$

To calculate one matrix element $S_{\alpha\beta}(\mathbf{k}, \omega)$ of the Green's function one must solve a set of $2n$ non-linear equations. When n is not small this procedure is not very convenient. Indeed, most of the calculations in the SDA have been restricted to the case of two poles. In the n-pole approximation we only need to find the roots of the characteristic polynomial of the energy matrix. Once the energy spectra $E_i(\mathbf{k})$ are calculated, the $n \times n$ Green's function can be immediately computed, as we have previously shown.

In conclusion, in this paper we have presented a general formulation based on the n-pole expansion for the calculation of the "single-particle" Green's function. The denomination "single-particle" is used in a generalized sense, and refers to the propagator of the n-component composite field $\{\psi_i\}$. Without recurring to a specific model, we have presented a scheme of calculations which allows us to determine the Green's function once the energy matrix $\epsilon(\mathbf{k})$ is known. This is the fundamental quantity and contains the dynamics, controlled by the Hamiltonian, the algebra, determined by the statistics of the original fields $\{\phi_i\}$, the boundary conditions, since it refers to expectation values. The conservation of the spectral moments has been analyzed. We have shown that there is an internal consistency in the n-pole approximation, in the sense that the exact relation between the spectral density function and the spectral moments, when calculated on the same ground, is preserved at any order. We have demonstrated a theorem that states that the full spectral moments, calculated on the basis of the exact Heisenberg equations, are conserved up to a certain order that depends on the number of poles. For example, in tha case of a single-band electron model, the spectral moments of the electronic field are conserved up to the $2n$th order. The method is equivalent to the spectral density approach. One advantage of this formulation with respect to the SDA is that we only need to solve the characteristic equation of $\epsilon(\mathbf{k})$.

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[9] Derivative operators $\lambda(-i\vec{\nabla})$ are defined as $\lambda(-i\vec{\nabla})f(\mathbf{x}) = \int d^d y \lambda(\mathbf{x}, \mathbf{y} f(\mathbf{y})$.

[10] For the sake of simplicity we are assuming translational invariance.

[11] A. Avella, F. Mancini, D. Villani, L. Siurakshina and V. Yu Yushankhai, *The Hubbard model in the two-pole approximation*, cond-mat/9708009 Int. Journ. Mod. Phys. B (in print).

[12] For example, let us consider the Hubbard model described by the Hamiltonian $H = \sum_{ij} c^{\dagger}(i)c(j) + U \sum_i n_{\uparrow}(i)n_{\downarrow}(i)$, where $c(i)$ is the electron field and we are using the standard notation. In the 3-pole approximation the choice $\psi(i) = \begin{pmatrix} c(i) \\ \eta(i) \\ \pi(i) \end{pmatrix}$ for the basic set, where $\eta(i) - n(i)c(i)$ and $\pi(i) = [\eta(i), H] - U\eta(i)$, $n(i)$ being the density operator, will ensure that the first 6 moments relative to the electron field $c(i)$ and the first 4 moments relative to the Hubbard field $\eta(i)$ are fully conserved.